Rational Modeling of Spectral Data using Orthorormal Vector Fitting

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Abstract
Vector Fitting (VF) is an iterative rational macromodeling technique [1] that became quite popular over the last years, due to its simplicity and availability. Although the VF method provides accurate broadband macromodels, the numerical stability of the algorithm is not always optimal. In this paper, the Orthorormal Vector Fitting (OVF) algorithm is introduced, which reduces the numerical sensitivity of the model parameterization to the choice of starting poles significantly, and limits the number of required iterations.

Introduction
Compact rational macromodels, based on measurements or simulations, are very important for efficient time domain and frequency domain simulation of high-speed interconnection structures.

Traditionally, a Vandermonde-like system of equations needs to be solved, in order to determine the system parameters of the rational macromodel. This approach, based on power series, is quite straightforward, but its accuracy is limited. The use of alternative polynomial bases, e.g. orthogonal Chebyshev polynomials of the first kind [4], is well-described in literature, but this approach doesn’t resolve all numerical issues.

Quite recently in 1999, an iterative least-squares approach (called Vector Fitting) [1], was proposed by Gustavsen and Semljen, which is essentially a reformulation of the Sanathanan-Koerner iteration [2] with rational basis functions. A detailed analysis and a more general framework of the iterative behaviour and convergence properties of the algorithm is discussed in [3]. This paper, will focus on improvements of the numerical stability and robustness of the VF algorithm. It will be shown that several numerical aspects of Vector Fitting can be improved when orthonormal rational functions are used. This reduces the numerical sensitivity of the model parameterization to the choice of the (starting) poles significantly, and can provide accurate macromodels in fewer iterations.

1 Rational approximation of data
A Linear Time-Invariant (LTI) system can be characterized in the frequency domain by fitting the spectral data to a rational macromodel in a least squares sense.

\[ R(s) = \frac{N(s)}{D(s)} = \frac{N_0 + \sum_{n=1}^{N} N_n \varphi_n(s)}{D_0 + \sum_{d=1}^{D} D_d \varphi_d(s)} \]  

(3)

In order to obtain a proper rational function \( R(s) \), the rational basis functions must span the space \( \mathcal{L}_n \), which is defined as

\[ \mathcal{L}_n = \text{span}\{ \varphi_0(s), \ldots, \varphi_p(s) \} \]

\[ \mathcal{L}_n = \left\{ \frac{p_n(s)}{\pi_n(s)} : p_n \in \Pi_n, \pi_n(s) = \prod_{p=1}^{P} (s + a_p) \right\} \]

(4)

(5)

where \( \Pi_n \) denotes the space of polynomials of degree equal to or less than \( n \) and \( a_n \) are chosen to be the poles of the rational basis functions, and \( \varphi_0(s) \) is assumed to be a constant function. Since \( R(s) \) represents a ratio of two rational functions (3), of which the poles of both the numerator and denominator lie in the same root of \( \varphi_n(s) \), they are cancelled out when the formulation is simplified and a representation as in (1) is obtained. This approach has several numerical advantages as will be shown further on. First, let’s focus on the identification of the system variables. The major difficulty with least-squares rational approximation is that the problem is still non-linear in terms of \( N_n \) and \( D_n \). One option, which is common in the engineering world, is to linearize the problem by multiplying left hand side and right hand side of (3) with the denominator expression. Hence, the following set of equations is obtained \( (D_0 = 1) \)

\[ \sum_{n=0}^{N} N_n \varphi_n(s) - R(s) \left( \sum_{d=1}^{D} D_d \varphi_d(s) \right) = R(s) \]

(6)
Note that this system of equations (evaluated at all discrete frequencies \( s \)) is no longer Vandermonde-like if the \( \varphi(s) \) are rational. In fact, when these basis functions are chosen carefully, the model parameterization is significantly better conditioned. This will become clear when we compare this "linearized least-squares" formulation to the Vector Fitting technique in the next paragraph.

2 Vector Fitting technique

The Vector Fitting technique approximates the frequency response with a rational pole-residue model \( R(s) \).

\[
R(s) = \sum_{p=1}^{P} \frac{c_p}{s + \alpha_p} + c_0
\]

(7)

\( R(s) \) approximates the simulated data samples at the discrete complex frequencies \( s \). \(-\alpha_p\) and \( c_p \) are the poles and residues respectively, \( \forall p = 1, \ldots, P \) and \( c_0 \) is a constant. The "weighted" data is approximated by a rational function \( \tilde{R}(s) \) based on an initial set of starting poles \( -\tilde{\alpha}_p \).

\[
\tilde{R}(s) = \sum_{p=1}^{P} \frac{\tilde{c}_p}{s + \tilde{\alpha}_p} + c_0
\]

(8)

This rational function approximates equation (7) multiplied by an unknown rational "weighting" function \( \sigma(s) \). Since \( \sigma(s) \) is also rational, it can be represented in pole-residue form, which leads to the following augmented problem

\[
\begin{bmatrix}
\sigma(s) R(s) \\
\sigma(s)
\end{bmatrix} = \begin{bmatrix}
\sum_{p=1}^{P} \frac{c_p}{s + \alpha_p} + c_0 \\
\sum_{p=1}^{P} \frac{\tilde{c}_p}{s + \tilde{\alpha}_p} + 1
\end{bmatrix}
\]

(9)

The augmented problem can be linearized in terms of the unknowns \( c_p, \tilde{c}_p, \alpha_p \) and \( \tilde{\alpha}_p \) by multiplying the second line of the vector equation with \( R(s) \).

\[
\left( \sum_{p=1}^{P} \frac{c_p}{s + \alpha_p} + c_0 \right) = \left( \sum_{p=1}^{P} \frac{\tilde{c}_p}{s + \tilde{\alpha}_p} + 1 \right) R(s)
\]

(10)

or

\[
(\sigma R)_{f, i}(s) = \sigma_{f, i}(s) R(s)
\]

(11)

Hence, the following set of linear equations is obtained

\[
\sum_{p=1}^{P} \frac{c_p}{s + \alpha_p} + c_0 - R(s) \left( \sum_{p=1}^{P} \frac{\tilde{c}_p}{s + \tilde{\alpha}_p} \right) = R(s)
\]

(12)

Remark that this form reduces exactly to (6)

\[
\sum_{p=0}^{P} c_p \varphi_p(s) - R(s) \left( \sum_{p=1}^{P} \tilde{c}_p \varphi_p(s) \right) = R(s)
\]

(13)

when the \( \varphi_p(s) \) are chosen to be the basis functions of the partial fraction expansion of a rational function.

\[
\varphi_0(s) = 1, \varphi_p(s) = \frac{1}{s + \alpha_p}
\]

(14)

Once the unknown parameters are estimated, \( R(s) \) can easily be obtained as

\[
R(s) = \frac{\sum_{p=0}^{P} c_p \varphi_p(s)}{\sum_{p=0}^{P} \tilde{c}_p \varphi_p(s)}
\]

(15)

Similarly, this ratio of rational functions with common denominator reduces after simplification to the classical pole-residue form (7) or the ratio of polynomials (3). The main conclusion of this paragraph is that the so-called "pole identification" of Vector Fitting reduces exactly to an iterative version of the "linearized least squares" formulation in the previous paragraph.

Note that the basis functions, chosen in the Vector Fitting technique, are the classical partial fraction expansion of a rational model. These basis functions are mainly responsible for the conditioning of the Vector Fitting technique, since they occur directly in the equations that need to be solved. In the next paragraph, it will be shown that alternative basis functions can be used as well.

3 The use of alternative basis functions

Instead of using the partial fractions as rational basis functions, it will be shown that orthonormal rational basis functions can lead to significant improvements in numerical conditioning [5]. A straightforward way to calculate an orthonormal basis, is to apply a Gram-Schmidt procedure on the partial fractions [6][7]. Hence, orthonormal rational functions \( \phi_p(s) \) are obtained, which are in fact linear combinations of the partial fractions \( \varphi_p(s) \), of the form

\[
\phi_p(s) = \frac{Q_p(s)}{\prod_{j=1}^{P} (s + a_j)}
\]

(16)

for \( p = 1, \ldots, P \) and \( Q_p(s) \) an arbitrary polynomial of order \( p - 1 \).

\[
\langle \phi_i(s), \phi_j(s) \rangle = \delta_{ij}
\]

(17)

The inner product is defined as

\[
\langle \phi_i(s), \phi_j(s) \rangle = \frac{1}{2\pi i} \int_{i\mathbb{R}} \phi_i(s) \phi_j^*(s) ds
\]

(18)

As an example, consider the construction of the first function \( \phi_1(s) \).

\[
\langle \phi_1(s), \phi_1(s) \rangle = \frac{1}{2\pi i} \int_{i\mathbb{R}} \phi_1(s) \phi_1^*(s) ds
\]

(19)

\[
= \frac{1}{2\pi i} \int_{i\mathbb{R}} \frac{|\gamma_1|^2}{(s + a_1)(-s + a_1^*)} ds
\]

(20)

\[
= \frac{|\gamma_1|^2}{a_1 + a_1^*}
\]

(21)

To normalize \( \phi_1(s) \), \( Q_1(s) = \gamma_1 \) must equal \( \kappa_1 \sqrt{2\text{Re}(a_1)} \), where \( \kappa_1 \) is an arbitrary unit-modulus complex number. \( \phi_1(s) \) is then obtained as

\[
\phi_1(s) = \kappa_1 \sqrt{2\text{Re}(a_1)} \frac{1}{s + a_1}
\]

(22)
Now consider the construction of the second function $\phi_2(s)$. First of all, $\phi_2(s)$ must be orthogonal to $\phi_1(s)$

$$\langle \phi_1(s), \phi_2(s) \rangle = \frac{1}{2\pi i} \int_{\mathbb{R}} \phi_1(s)\bar{\phi}_2(s) ds = 0$$

(23)

which implies that $\phi_2(s)$ must vanish for $s = -a_i$. Therefore $Q_2(s) = \gamma_2(s - a_i^*)$. This constant $\gamma_2$ is determined by imposing the normalization condition

$$\langle \phi_2(s), \phi_2(s) \rangle = \frac{1}{2\pi i} \int_{\mathbb{R}} \frac{\gamma_2(s - a_i^*)}{(s + a_i)(s + a_2^*)} \frac{\gamma_2^*(s - a_i)}{(s + a_i^*)(s + a_2)} ds$$

$$= \frac{1}{2\pi} \int_{\mathbb{R}} \frac{|\gamma_2|^2}{(s + a_2^*)(s + a_i^*)} ds = \frac{1}{2\pi} |\gamma_2|^2$$

(24)

Clearly, it follows that $\gamma_2 = \kappa_2 \sqrt{2\text{Re}(a_2)}$, where $\kappa_2$ is an arbitrary unimodular complex number. So, $\phi_2(s)$ is then given by

$$\phi_2(s) = \kappa_2 \sqrt{2\text{Re}(a_2)} \frac{s - a_i^*}{(s + a_i)(s + a_2)}$$

(25)

Similarly continuing this approach, the general polynomials obtained

$$\phi_p(s) = \kappa_p \left( \prod_{j=1}^{p-1} \frac{s - a_j^*}{s + a_j} \right) \sqrt{2\text{Re}(a_p)} \frac{1}{s + a_p}$$

(26)

The calculation of this basis is not new, but is given here for the sake of completeness and ease of understanding. In fact, orthogonal rational functions have a long history in mathematics and engineering. This basis originates from the discrete-time Takenaka-Malmquist basis [8]-[9], originally developed in 1925, and has later been transformed to the continuous time domain. It is a generalization of the Laguerre basis [10], where all polynomials $-a_p$ are the same real number, and the Kautz bases [11] where all polynomials $-a_p, -a_{p+1}$ are the same complex conjugate pair with $a_p^* = -a_{p+1}$.

For the macromodeling of LTI systems, the basis functions must have real coefficients, hence a linear combination of $\phi_i(s)$ and $\phi_i(s)$ is formed

$$\alpha \phi_i(s) + \beta \phi_i(s) = \left( \prod_{j=1}^{i-1} \frac{s - a_j^*}{s + a_j} \right) \frac{\alpha(s + a_{i+1}) + \beta(s - a_i^*)}{(s + a_i)(s + a_{i+1})}$$

(27)

which can be made real-valued if $a_{i+1} = a_i^*$ (or if both $a_i$ and $a_{i+1}$ are real). This way, two orthonormal functions of the following form are obtained

$$\phi_i(s) = \gamma_i \left( \prod_{j=1}^{i-1} \frac{s - a_j^*}{s + a_j} \right) \frac{s - x}{(s + a_i)(s + a_{i+1})}$$

(28)

$$\phi_{i+1}(s) = \gamma_{i+1} \left( \prod_{j=1}^{i-1} \frac{s - a_j^*}{s + a_j} \right) \frac{s - y}{(s + a_i)(s + a_{i+1})}$$

(29)

with real $\gamma_i, \gamma_{i+1}, x$ and $y$. To impose the orthogonality,

$$\langle \phi_i(s), \phi_{i+1}(s) \rangle = \gamma_i \gamma_{i+1} \frac{xy + a_i a_{i+1}}{2(a_i + a_{i+1}) a_i a_{i+1}} = 0$$

(30)

$x$ and $y$ are set to $\sqrt{a_i a_{i+1}}$ and $-\sqrt{a_i a_{i+1}}$ respectively. Similarly, $\gamma_i$ and $\gamma_{i+1}$ are set to $\sqrt{a_i a_{i+1}}$. Note that this choice is not unique, and that other possibilities exist.

Implementing these orthonormal rational basis functions in VF (see Section II and III) leads to OFV. The OFV technique makes the model parameterization significantly better conditioned, especially if the poles are real, or the magnitude of the real part of the complex poles is non-negligible. Unstable poles can either be flipped into the left half plane or deleted in each iteration. Passivity can be enforced as post-processing technique [13][14][15].

4 Example

The reflection coefficient $S_{11}$ of a Quarter Wave Filter (QWVL) is modeled over the frequency range of interest [1 GHz - 12 GHz], based on a set of 32 equidistant support samples. The initial poles are chosen as complex conjugate pairs (imaginary parts equidistantly spread over the frequency range of interest), with a fixed real part. Both techniques (VF and OFV) are used to fit the rational data using the same set of initial poles, and are allowed one single iteration. Table 1 shows the condition number of both techniques (ratio between largest and smallest singular value) when the real part of the poles varies from -1 to -5. Clearly, the new technique is significantly better conditioned when the distance between the poles and the imaginary axis increases. Fig. 1 shows both rational fits, and their corresponding error when the real part is set to -5. Fig. 2 shows the corresponding singular values of the "pole identification". Due to numerical problems, VF was unable to provide accurate results in only 1 iteration. Using OFV, on the other hand, numerical problems are avoided and the accuracy is almost twice as good. In general, the best results for both techniques are obtained when the initial poles are chosen as described in [1].

5 Conclusion

In this paper, the Vector Fitting technique is modified such that orthonormal rational functions are used during the fitting process. Several examples show that this approach improves the numerical conditioning of the pole-identification significantly. The Orthonormal Vector Fitting (OFV) technique can provide accurate results when the starting poles are not chosen optimally, often in fewer iterations.
Figure 1: Left: Magnitude $S_{11}$ of QWVL using VF (dashed) and OVF (full). Right: Accuracy of the fit.

<table>
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<tr>
<th>$\Re(-\alpha_p)$</th>
<th>Cond. Nr. VF</th>
<th>Cond. Nr. OVF</th>
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<tr>
<td>-5</td>
<td>$8.5856 \times 10^{14}$</td>
<td>$4.2810 \times 10^{11}$</td>
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<tr>
<td>-4</td>
<td>$5.4016 \times 10^{16}$</td>
<td>$2.3412 \times 10^{10}$</td>
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<td>-3</td>
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Table 1: Conditioning vs. pole location.

6 Acknowledgements
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References


